Microcystin LR

101043-37-2 | DTXSID3031654

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 343 °C

Global applicability domain: Outside

Local applicability domain index: 2.43e-02

Confidence level: 4.05e-01

Nearest Neighbors from the Training Set

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Aminotrimethylene phosphonic acid
Measured: 480
Predicted: 478

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Diphenylurea
Measured: 262
Predicted: 269

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N-(4-Bromophenyl)urea
Measured: 260
Predicted: 256

Image not found

Ametryn
Measured: 345
Predicted: 341

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Desmetryn
Measured: 345
Predicted: 341